Alexandre Varnek

List of Publications by Year
in descending order

220	9,116	61984	49909
papers	citations	43 h-index	87 g-index

242	242	242	6902
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	QSAR Modeling: Where Have You Been? Where Are You Going To?. Journal of Medicinal Chemistry, 2014, 57, 4977-5010.	6.4	1,401
2	Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. Journal of Computer-Aided Molecular Design, 2011, 25, 533-554.	2.9	453
3	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	38.1	427
4	Critical Assessment of QSAR Models of Environmental Toxicity against Tetrahymena pyriformis: Focusing on Applicability Domain and Overfitting by Variable Selection. Journal of Chemical Information and Modeling, 2008, 48, 1733-1746.	5.4	350
5	Estimation of the size of drug-like chemical space based on GDB-17 data. Journal of Computer-Aided Molecular Design, 2013, 27, 675-679.	2.9	319
6	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	6.0	264
7	Combinatorial QSAR Modeling of Chemical Toxicants Tested against Tetrahymena pyriformis. Journal of Chemical Information and Modeling, 2008, 48, 766-784.	5.4	258
8	Applicability Domains for Classification Problems: Benchmarking of Distance to Models for Ames Mutagenicity Set. Journal of Chemical Information and Modeling, 2010, 50, 2094-2111.	5.4	202
9	Machine Learning Methods for Property Prediction in Chemoinformatics: Quo Vadis?. Journal of Chemical Information and Modeling, 2012, 52, 1413-1437.	5.4	191
10	ISIDA - Platform for Virtual Screening Based on Fragment and Pharmacophoric Descriptors. Current Computer-Aided Drug Design, 2008, 4, 191-198.	1.2	173
11	Substructural fragments: an universal language to encode reactions, molecular and supramolecular structures. Journal of Computer-Aided Molecular Design, 2005, 19, 693-703.	2.9	166
12	Predicting the Predictability: A Unified Approach to the Applicability Domain Problem of QSAR Models. Journal of Chemical Information and Modeling, 2009, 49, 1762-1776.	5.4	145
13	Exhaustive QSPR Studies of a Large Diverse Set of Ionic Liquids:â€‰ How Accurately Can We Predict Melting Points?. Journal of Chemical Information and Modeling, 2007, 47, 1111-1122.	5.4	129
14	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	38.1	128
15	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	6.0	120
16	ISIDA Propertyâ€Labelled Fragment Descriptors. Molecular Informatics, 2010, 29, 855-868.	2.5	111
17	Generative Topographic Mapping (GTM): Universal Tool for Data Visualization, Structureâ€Activity Modeling and Dataset Comparison. Molecular Informatics, 2012, 31, 301-312.	2.5	107
18	De Novo Molecular Design by Combining Deep Autoencoder Recurrent Neural Networks with Generative Topographic Mapping. Journal of Chemical Information and Modeling, 2019, 59, 1182-1196.	5.4	93

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19	Molecular dynamics study of p-tert-butylcalix[4]arenetetraamide and its complexes with neutral and cationic guests. Influence of solvation on structures and stabilities. Journal of the American Chemical Society, 1993, 115, 8298-8312.	13.7	82
20	Correlation of bloodâ€“brain penetration using structural descriptors. Bioorganic and Medicinal Chemistry, 2006, 14, 4888-4917.	3.0	80
21	Chemoinformatics as a Theoretical Chemistry Discipline. Molecular Informatics, 2011, 30, 20-32.	2.5	78
22	Modeling of Ion Complexation and Extraction Using Substructural Molecular Fragments. Journal of Chemical Information and Computer Sciences, 2000, 40, 847-858.	2.8	76
23	Inductive Transfer of Knowledge: Application of Multi-Task Learning and Feature Net Approaches to Model Tissue-Air Partition Coefficients. Journal of Chemical Information and Modeling, 2009, 49, 133-144.	5.4	71
24	Benchmarking of Linear and Nonlinear Approaches for Quantitative Structureâ^'Property Relationship Studies of Metal Complexation with Ionophores. Journal of Chemical Information and Modeling, 2006, 46, 808-819.	5.4	68
25	Chemical Data Visualization and Analysis with Incremental Generative Topographic Mapping: Big Data Challenge. Journal of Chemical Information and Modeling, 2015, 55, 84-94.	5.4	67
26	Quantitative Structureâ^'Property Relationship Modeling ofÎ²-Cyclodextrin Complexation Free Energies. Journal of Chemical Information and Computer Sciences, 2004, 44, 529-541.	2.8	66
27	Expert System for Predicting Reaction Conditions: The Michael Reaction Case. Journal of Chemical Information and Modeling, 2015, 55, 239-250.	5.4	65
28	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	6.0	63
29	QSPR Approach to Predict Nonadditive Properties of Mixtures. Application to Bubble Point Temperatures of Binary Mixtures of Liquids. Molecular Informatics, 2012, 31, 491-502.	2.5	59
30	Theoretical calculations of extraction selectivity: Alkali cation complexes of calix[4]-bis-crown6 in pure water, chloroform, and at a water/chloroform interface. Journal of Computational Chemistry, 1996, 17, 1520-1531.	3.3	58
31	Generative Topographic Mapping-Based Classification Models and Their Applicability Domain: Application to the Biopharmaceutics Drug Disposition Classification System (BDDCS). Journal of Chemical Information and Modeling, 2013, 53, 3318-3325.	5.4	55
32	Evolution of commercially available compounds for HTS. Drug Discovery Today, 2019, 24, 390-402.	6.4	53
33	An Evolutionary Optimizer of libsvm Models. Challenges, 2014, 5, 450-472.	1.7	52
34	Mappability of drug-like space: towards a polypharmacologically competent map of drug-relevant compounds. Journal of Computer-Aided Molecular Design, 2015, 29, 1087-1108.	2.9	52
35	GTMâ€Based QSAR Models and Their Applicability Domains. Molecular Informatics, 2015, 34, 348-356.	2.5	52
36	Integrated Strategy for Lead Optimization Based on Fragment Growing: The Diversity-Oriented-Target-Focused-Synthesis Approach. Journal of Medicinal Chemistry, 2018, 61, 5719-5732.	6.4	51

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37	Skin Permeation Rate as a Function of Chemical Structure. Journal of Medicinal Chemistry, 2006, 49, 3305-3314.	6.4	49
38	The Oneâ€Class Classification Approach to Data Description and to Models Applicability Domain. Molecular Informatics, 2010, 29, 581-587.	2.5	49
39	In Silico Design of New Ionic Liquids Based on Quantitative Structureâ^'Property Relationship Models of Ionic Liquid Viscosity. Journal of Physical Chemistry B, 2011, 115, 93-98.	2.6	48
40	Predicting Ligand Binding Modes from Neural Networks Trained on Proteinâ€"Ligand Interaction Fingerprints. Journal of Chemical Information and Modeling, 2013, 53, 763-772.	5.4	47
41	Solvent and counterion effects on complexation selectivity by conformationally locked calix[4]-bis-crown ligands: Molecular Dynamics and Free Energy Perturbation studies in water and methanol, acetonitrile and chloroform solutions. Computational and Theoretical Chemistry, 1996, 363, 67-85.	1.5	45
42	New organophosphorus calix[4]arene ionophores for trivalent lanthanide and actinide cations. Journal of Supramolecular Chemistry, 2002, 2, 421-427.	0.4	45
43	Artificial intelligence in synthetic chemistry: achievements and prospects. Russian Chemical Reviews, 2017, 86, 1127-1156.	6.5	45
44	â€œIn Silicoâ€•Design of New Uranyl Extractants Based on Phosphoryl-Containing Podands:â€‰ QSPR Studies, Generation and Screening of Virtual Combinatorial Library, and Experimental Tests. Journal of Chemical Information and Computer Sciences, 2004, 44, 1365-1382.	2.8	44
45	New Wide Rim Phosphomethylated Calix[4]arenes in Extraction of Americium and Europium. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2004, 49, 47-56.	1.6	43
46	Dramatic solvent effect on the ligand wrapping around a complexed cation: a MD study of p-tert-butylcalix[4]arene tetramide and its complexes with alkali cations and europium(3+) in acetonitrile. The Journal of Physical Chemistry, 1993, 97, 10840-10848.	2.9	41
47	Assessment of the Macrocyclic Effect for the Complexation of Crown-Ethers with Alkali Cations Using the Substructural Molecular Fragments Method. Journal of Chemical Information and Computer Sciences, 2002, 42, 812-829.	2.8	41
48	QSAR modeling of blood:air and tissue:air partition coefficients using theoretical descriptors. Bioorganic and Medicinal Chemistry, 2005, 13, 6450-6463.	3.0	40
49	Discovery of novel chemical reactions by deep generative recurrent neural network. Scientific Reports, 2021, 11, 3178.	3.3	40
50	Anti-HIV Activity of HEPT, TIBO, and Cyclic Urea Derivatives:â€‰ Structureâ^'Property Studies, Focused Combinatorial Library Generation, and Hits Selection Using Substructural Molecular Fragments Method. Journal of Chemical Information and Computer Sciences, 2003, 43, 1703-1719.	2.8	39
51	A REPRESENTATION TO APPLY USUAL DATA MINING TECHNIQUES TO CHEMICAL REACTIONS â€" ILLUSTRATION ON THE RATE CONSTANT OF S_{N}2 REACTIONS IN WATER. International Journal on Artificial Intelligence Tools, 2011, 20, 253-270.	1.0	39
52	Automatized Assessment of Protective Group Reactivity: A Step Toward Big Reaction Data Analysis. Journal of Chemical Information and Modeling, 2016, 56, 2140-2148.	5.4	37
53	Complexation of the p-t-butyl-calix[4]arene anion with alkali metal cations in polar, non-aqueous solvents: experimental and theoretical studies. Inorganica Chimica Acta, 1996, 246, 275-286.	2.4	35
54	Electrochemical Properties of Substituted 2â€Methylâ€1,4â€Naphthoquinones: Redox Behavior Predictions. Chemistry - A European Journal, 2015, 21, 3415-3424.	3.3	35

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55	Structural and Physico-Chemical Interpretation (SPCI) of QSAR Models and Its Comparison with Matched Molecular Pair Analysis. Journal of Chemical Information and Modeling, 2016, 56, 1455-1469.	5.4	35
56	CGRtools: Python Library for Molecule, Reaction, and Condensed Graph of Reaction Processing. Journal of Chemical Information and Modeling, 2019, 59, 2516-2521.	5.4	34
57	Mapping of the Available Chemical Space versus the Chemical Universe of Leadâ€Like Compounds. ChemMedChem, 2018, 13, 540-554.	3.2	33
58	Stochastic versus Stepwise Strategies for Quantitative Structureâ^'Activity Relationship GenerationHow Much Effort May the Mining for Successful QSAR Models Take?. Journal of Chemical Information and Modeling, 2007, 47, 927-939.	5.4	32
59	Interpretability of SAR/QSAR Models of any Complexity by Atomic Contributions. Molecular Informatics, 2012, 31, 639-642.	2.5	32
60	Comprehensive Analysis of Applicability Domains of QSPR Models for Chemical Reactions. International Journal of Molecular Sciences, 2020, 21, 5542.	4.1	32
61	A Close-up Look at the Chemical Space of Commercially Available Building Blocks for Medicinal Chemistry. Journal of Chemical Information and Modeling, 2022, 62, 2171-2185.	5.4	32
62	Chemical Space Mapping and Structureâ€“Activity Analysis of the ChEMBL Antiviral Compound Set. Journal of Chemical Information and Modeling, 2016, 56, 1438-1454.	5.4	31
63	Adsorption of Ionophores and of Their Cation Complexes at the Water/Chloroform Interface: A Molecular Dynamics Study of a [2.2.2]Cryptand and of Phosphorylâ€Containing Podands. Chemistry - A European Journal, 1997, 3, 552-560.	3.3	29
64	Design of a Generalâ€Purpose European Compound Screening Library for EUâ€OPENSCREEN. ChemMedChem, 2014, 9, 2309-2326.	3.2	29
65	Structure-reactivity relationships in terms of the condensed graphs of reactions. Russian Journal of Organic Chemistry, 2014, 50, 459-463.	0.8	29
66	Upper Rim Thioether Derivatives of Calix[4,6]Arenes: Extraction of Fission Pd(II) and Ag(I). Solvent Extraction and Ion Exchange, 2005, 23, 781-801.	2.0	28
67	Recovery of uranium (VI) from concentrated phosphoric acid by mixtures of new bis(1,3-) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 28-33.	4.3	28
68	Stargate GTM: Bridging Descriptor and Activity Spaces. Journal of Chemical Information and Modeling, 2015, 55, 2403-2410.	5.4	28
69	Prediction of Activity Cliffs Using Condensed Graphs of Reaction Representations, Descriptor Recombination, Support Vector Machine Classification, and Support Vector Regression. Journal of Chemical Information and Modeling, 2016, 56, 1631-1640.	5.4	28
70	Redox Polypharmacology as an Emerging Strategy to Combat Malarial Parasites. ChemMedChem, 2016, 11, 1339-1351.	3.2	28
71	Structureâ€"property modeling of metal binders using molecular fragments. Russian Chemical Bulletin, 2004, 53, 1434-1445.	1.5	27
72	Transductive Support Vector Machines: Promising Approach to Model Small and Unbalanced Datasets. Molecular Informatics, 2013, 32, 261-266.	2.5	26

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73	Computational chemogenomics: Is it more than inductive transfer?. Journal of Computer-Aided Molecular Design, 2014, 28, 597-618.	2.9	26
74	Quantitative Structureâ€“Property Relationship (QSPR) Modeling of Normal Boiling Point Temperature and Composition of Binary Azeotropes. Industrial & Engineering Chemistry Research, 2011, 50, 14162-14167.	3.7	25
75	Simple Ligandâ€“Receptor Interaction Descriptor (SILIRID) for alignment-free binding site comparison. Computational and Structural Biotechnology Journal, 2014, 10, 33-37.	4.1	25
76	S4MPLEâ€”Sampler for Multiple Protein-Ligand Entities: Methodology and Rigid-Site Docking Benchmarking. Molecules, 2015, 20, 8997-9028.	3.8	25
77	Structureâ€“reactivity relationship in bimolecular elimination reactions based on the condensed graph of a reaction. Journal of Structural Chemistry, 2015, 56, 1227-1234.	1.0	25
78	Predictive Models for Kinetic Parameters of Cycloaddition Reactions. Molecular Informatics, 2019, 38, e1800077.	2.5	25
79	Prediction of the Glass-Transition Temperatures of Linear Homo/Heteropolymers and Cross-Linked Epoxy Resins. ACS Applied Polymer Materials, 2019, 1, 1430-1442.	4.4	25
80	Successful â€œIn Silicoâ€•Design of New Efficient Uranyl Binders. Solvent Extraction and Ion Exchange, 2007, 25, 433-462.	2.0	24
81	Mining Chemical Reactions Using Neighborhood Behavior and Condensed Graphs of Reactions Approaches. Journal of Chemical Information and Modeling, 2012, 52, 2325-2338.	5.4	24
82	Structureâ€“reactivity modeling using mixture-based representation of chemical reactions. Journal of Computer-Aided Molecular Design, 2017, 31, 829-839.	2.9	23
83	Bimolecular Nucleophilic Substitution Reactions: Predictive Models for Rate Constants and Molecular Reaction Pairs Analysis. Molecular Informatics, 2019, 38, e1800104.	2.5	23
84	Prediction of Drug Induced Liver Injury Using Molecular and Biological Descriptors. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 315-322.	1.1	23
85	TOWARDS AN INFORMATION SYSTEM ON SOLVENT EXTRACTION. Solvent Extraction and Ion Exchange, 2001, 19, 791-837.	2.0	22
86	Design, Virtual Screening, and Synthesis of Antagonists of Î±_{IIb}Î²₃ as Antiplatelet Agents. Journal of Medicinal Chemistry, 2015, 58, 7681-7694.	6.4	22
87	Consensus models to predict oral rat acute toxicity and validation on a dataset coming from the industrial context. SAR and QSAR in Environmental Research, 2019, 30, 879-897.	2.2	22
88	QSPR Modeling of the AmIII/EuIIISeparation Factor: How Far Can we Predict ?. Solvent Extraction and Ion Exchange, 2007, 25, 1-26.	2.0	21
89	Synthesis and structure of heterometallic compounds of [RuNO(NO2)4OH]2â^' with triphenyl phosphine oxide complexes of Co(II), Ni (II), and Zn(II). Journal of Molecular Structure, 2007, 837, 63-71.	3.6	21
90	QSPR ensemble modelling of alkaline-earth metal complexation. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2013, 76, 159-171.	1.6	21

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91	New Approach for Accurate QSPR Modeling of Metal Complexation: Application to Stability Constants of Complexes of Lanthanide Ions Ln3+, Ag+, Zn2+, Cd2+ and Hg2+ with Organic Ligands in Water. Macroheterocycles, 2012, 5, 404-410.	0.5	21
92	Models for Identification of Erroneous Atom-to-Atom Mapping of Reactions Performed by Automated Algorithms. Journal of Chemical Information and Modeling, 2012, 52, 3116-3122.	5.4	20
93	Assessment of tautomer distribution using the condensed reaction graph approach. Journal of Computer-Aided Molecular Design, 2018, 32, 401-414.	2.9	20
94	Serum-based differentiation between multiple sclerosis and amyotrophic lateral sclerosis by Random Forest classification of FTIR spectra. Analyst, The, 2019, 144, 4647-4652.	3.5	20
95	Virtual Screening with Generative Topographic Maps: How Many Maps Are Required?. Journal of Chemical Information and Modeling, 2019, 59, 564-572.	5.4	20
96	Stability constants of complexes of Zn2+, Cd2+, and Hg2+ with organic ligands: QSPR consensus modeling and design of new metal binders. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2012, 72, 309-321.	1.6	19
97	Do Not Hesitate to Use Tverskyâ€"and Other Hints for Successful Active Analogue Searches with Feature Count Descriptors. Journal of Chemical Information and Modeling, 2013, 53, 1543-1562.	5.4	19
98	QSPR ensemble modelling of the 1:1 and 1:2 complexation of Co2+, Ni2+, and Cu2+ with organic ligands: relationships between stability constants. Journal of Computer-Aided Molecular Design, 2014, 28, 549-564.	2.9	19
99	Individual Hydrogenâ€Bond Strength QSPR Modelling with ISIDA Local Descriptors: a Step Towards Polyfunctional Molecules. Molecular Informatics, 2014, 33, 477-487.	2.5	19
100	Generative topographic mapping in drug design. Drug Discovery Today: Technologies, 2019, 32-33, 99-107.	4.0	19
101	Consensus QSAR models estimating acute toxicity to aquatic organisms from different trophic levels: algae, Daphnia and fish. SAR and QSAR in Environmental Research, 2020, 31, 655-675.	2.2	19
102	SOLVENT EXTRACTION OF METAL PICRATES BY PHOSPHORYL-CONTAINING PODANDS. Solvent Extraction and Ion Exchange, 1999, 17, 495-523.	2.0	18
103	“In Silico” Design of Potential Anti-HIV Actives Using Fragment Descriptors. Combinatorial Chemistry and High Throughput Screening, 2005, 8, 403-416.	1.1	18
104	Quantitative Structureâ€"Property Relationship Modeling: A Valuable Support in High-Throughput Screening Quality Control. Analytical Chemistry, 2014, 86, 2510-2520.	6.5	18
105	QSPR models for bioconcentration factor (BCF): are they able to predict data of industrial interest?. SAR and QSAR in Environmental Research, 2019, 30, 507-524.	2.2	18
106	SynthI: A New Open-Source Tool for Synthon-Based Library Design. Journal of Chemical Information and Modeling, 2022, 62, 2151-2163.	5.4	18
107	van der Waals host-guest complexes: Can one predict complexation selectivity of neutral guests by a cryptophane? MD-FEP studies in gas phase and chloroform solution. Journal of Computational Chemistry, 1998, 19, 820-832.	3.3	17
108	Complexes of the H5O2+ and H3O+ cations with polyethers in water saturated dichloroethane solutions. A combined IR spectroscopic and quantum mechanics studyElectronic supplementary information (ESI) available: the coordinates of the 6-31G* optimized systems (four files in PDB format). See http://www.rsc.org/suppdata/p2/b2/b201034h/. Perkin Transactions II RSC, 2002, , 887-893.	1.1	17

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109	Building a Chemical Space Based on Fragment Descriptors. Combinatorial Chemistry and High Throughput Screening, 2008, 11, 661-668.	1.1	17
110	Using self-organizing maps to accelerate similarity search. Bioorganic and Medicinal Chemistry, 2012, 20, 5396-5409.	3.0	17
111	Multi-task generative topographic mapping in virtual screening. Journal of Computer-Aided Molecular Design, 2019, 33, 331-343.	2.9	17
112	Atomâ€toâ€atom Mapping: A Benchmarking Study of Popular Mapping Algorithms and Consensus Strategies. Molecular Informatics, 2022, 41, e2100138.	2.5	17
113	Computational screening methodology identifies effective solvents for CO2 capture. Communications Chemistry, 2022, 5, .	4.5	17
114	Structure-property modelling of complex formation of strontium with organic ligands in water. Journal of Structural Chemistry, 2006, 47, 298-311.	1.0	16
115	Complexation of Mn²⁺, Fe²⁺, Y³⁺, La³⁺, Pb²⁺, and UO₂²⁺ with Organic Ligands: QSPR Ensemble Modeling of Stability Constants. Industrial & Engineering Chemistry Research, 2012, 51, 13482-13489.	3.7	16
116	In Silico Mining for Antimalarial Structure-Activity Knowledge and Discovery of Novel Antimalarial Curcuminoids. Molecules, 2016, 21, 853.	3.8	16
117	A Chemographic Audit of antiâ€Coronavirus Structureâ€activity Information from Public Databases (ChEMBL). Molecular Informatics, 2020, 39, e2000080.	2.5	16
118	NP Navigator: A New Look at the Natural Product Chemical Space. Molecular Informatics, 2021, 40, e2100068.	2.5	16
119	Chemoinformatics-Driven Design of New Physical Solvents for Selective CO₂ Absorption. Environmental Science & Technology, 2021, 55, 15542-15553.	10.0	16
120	Development of â€œstructure-propertyâ€•models in nucleophilic substitution reactions involving azides. Journal of Structural Chemistry, 2014, 55, 1026-1032.	1.0	15
121	Generative Topographic Mapping Approach to Chemical Space Analysis. ACS Symposium Series, 2016, , 211-241.	0.5	15
122	Virtual screening, synthesis and biological evaluation of DNA intercalating antiviral agents. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 3915-3919.	2.2	15
123	Rescoring of docking poses under Occamâ€™s Razor: are there simpler solutions?. Journal of Computer-Aided Molecular Design, 2018, 32, 877-888.	2.9	15
124	Reaction Data Curation I: Chemical Structures and Transformations Standardization. Molecular Informatics, 2021, 40, e2100119.	2.5	15
125	QSAR Modeling Based on Conformation Ensembles Using a Multi-Instance Learning Approach. Journal of Chemical Information and Modeling, 2021, 61, 4913-4923.	5.4	15
126	Molecular modelling of organophosphorus podands and their complexes with alkali metal cations. Journal of Physical Organic Chemistry, 1992, 5, 109-118.	1.9	14

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127	The structure of new heterometallic Ru/M (M=Cu, Ni, Co, Zn) complexes investigated by combined spectroscopic and modeling studies. Journal of Molecular Structure, 2002, 611, 131-138.	3.6	14
128	Electronic, Spectroscopic, and Ion-Sensing Properties of a Dehydro[m]pyrido[14]- and [15]annulene Isomer Library. Journal of Organic Chemistry, 2012, 77, 126-142.	3.2	14
129	Kernel Target Alignment Parameter: A New Modelability Measure for Regression Tasks. Journal of Chemical Information and Modeling, 2016, 56, 6-11.	5.4	14
130	Modelling of ready biodegradability based on combined public and industrial data sources. SAR and QSAR in Environmental Research, 2020, 31, 171-186.	2.2	14
131	Chemography: Searching for Hidden Treasures. Journal of Chemical Information and Modeling, 2021, 61, 179-188.	5.4	14
132	Computer-aided design of new metal binders. Radiochimica Acta, 2008, 96, 505-511.	1.2	13
133	QSAR modeling and chemical space analysis of antimalarial compounds. Journal of Computer-Aided Molecular Design, 2017, 31, 441-451.	2.9	13
134	CovaDOTS: In Silico Chemistry-Driven Tool to Design Covalent Inhibitors Using a Linking Strategy. Journal of Chemical Information and Modeling, 2019, 59, 1472-1485.	5.4	13
135	Theoretical ab initio and semiempirical studies on biologically important di- and oligopyrrolic compounds. Pyrromethenone and biliverdin. Computational and Theoretical Chemistry, 1998, 425, 137-145.	1.5	12
136	Predictive Models for Halogenâ€bond Basicity of Binding Sites of Polyfunctional Molecules. Molecular Informatics, 2016, 35, 70-80.	2.5	12
137	Pros and cons of virtual screening based on public â€œBig Dataâ€: In silico mining for new bromodomain inhibitors. European Journal of Medicinal Chemistry, 2019, 165, 258-272.	5.5	12
138	Cross-validation strategies in QSPR modelling of chemical reactions. SAR and QSAR in Environmental Research, 2021, 32, 207-219.	2.2	12
139	Quantitative Structure-Property Relationships in Solvent Extraction and Complexation of Metals. Ion Exchange and Solvent Extraction, 2009, , 319-358.	0.3	12
140	MOLECULAR MODELLING IN SOLVENT EXTRACTION: IONOPHORES IN PURE SOLUTIONS AND AT THE LIQUID/LIQUID INTERFACE. Solvent Extraction and Ion Exchange, 1999, 17, 1493-1505.	2.0	11
141	QSPR modeling of potentiometric sensitivity towards heavy metal ions for polymeric membrane sensors. Sensors and Actuators B: Chemical, 2019, 301, 126941.	7.8	11
142	Prediction of Optimal Salinities for Surfactant Formulations Using a Quantitative Structureâ€“Property Relationships Approach. Energy & Fuels, 2015, 29, 4281-4288.	5.1	10
143	Generative Topographic Mapping of Conformational Space. Molecular Informatics, 2017, 36, 1700036.	2.5	10
144	Synthesis and Extractive Properties of Hexaphosphorylated Calix[6]arenes. Russian Journal of General Chemistry, 2002, 72, 1736-1742.	0.8	9

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145	Local neighborhood behavior in a combinatorial library context. Journal of Computer-Aided Molecular Design, 2011, 25, 237-252.	2.9	9
146	Predictive Models for the Free Energy of Hydrogen Bonded Complexes with Single and Cooperative Hydrogen Bonds. Molecular Informatics, 2016, 35, 629-638.	2.5	9
147	Privileged Structural Motif Detection and Analysis Using Generative Topographic Maps. Journal of Chemical Information and Modeling, 2017, 57, 1218-1232.	5.4	9
148	QSPR Modeling of Potentiometric Mg²⁺/Ca²⁺ Selectivity for PVCâ€plasticized Sensor Membranes. Electroanalysis, 2020, 32, 792-798.	2.9	9
149	Computer-Aided Design of New Physical Solvents for Hydrogen Sulfide Absorption. Industrial & Engineering Chemistry Research, 2021, 60, 8588-8596.	3.7	9
150	Exploration of the Chemical Space of DNAâ€encoded Libraries. Molecular Informatics, 2022, 41, .	2.5	9
151	Machine learning modelling of chemical reaction characteristics: yesterday, today, tomorrow. Mendeleev Communications, 2021, 31, 769-780.	1.6	9
152	Complexation of lithium and sodium cations with Î²-phosphorylate ethers, modelling terminal groups of organophosphorus podands. An experimental and theoretical study. Journal of Molecular Structure, 1992, 271, 311-325.	3.6	8
153	Supramolecular Chemistry: Computer-Assisted Instruction in Undergraduate and Graduate Chemistry Courses. Journal of Chemical Education, 2000, 77, 222.	2.3	8
154	Synthesis of a Strained Acetylenic Macrocycle Incorporating a paraâ€Oligo[2]cruciform Bridge Bent over Nanoscopic Dimensions: Structural, Electronic, Spectroscopic, and Ionâ€Sensing Properties. Chemistry - A European Journal, 2013, 19, 12336-12349.	3.3	8
155	Visualization of a Multidimensional Descriptor Space. ACS Symposium Series, 2016, , 243-267.	0.5	8
156	Classification of Metal Binders by NaÃ¯ve Bayes Classifier on the Base of Molecular Fragment Descriptors and Ensemble Modeling. Molecular Informatics, 2019, 38, e1900002.	2.5	8
157	Application of the mol2vec Technology to Largeâ€size Data Visualization and Analysis. Molecular Informatics, 2020, 39, e1900170.	2.5	8
158	Multi-Instance Learning Approach to Predictive Modeling of Catalysts Enantioselectivity. Synlett, 2021, 32, 1833-1836.	1.8	8
159	Fragment Descriptors in Structureâ€“Property Modeling and Virtual Screening. Methods in Molecular Biology, 2010, 672, 213-243.	0.9	7
160	Synthesis, biological evaluation, X-ray molecular structure and molecular docking studies of RGD mimetics containing 6-amino-2,3-dihydroisoindolin-1-one fragment as ligands of integrin Î±IIbÎ²3. Bioorganic and Medicinal Chemistry, 2013, 21, 4646-4661.	3.0	7
161	Publicly available models to predict normal boiling point of organic compounds. Thermochimica Acta, 2013, 553, 60-67.	2.7	7
162	Visualization and Analysis of Complex Reaction Data: The Case of Tautomeric Equilibria. Molecular Informatics, 2018, 37, e1800056.	2.5	7

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